Journal of Materials Chemistry

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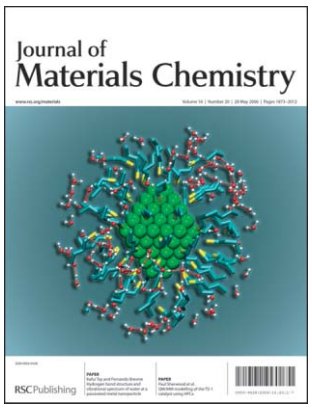
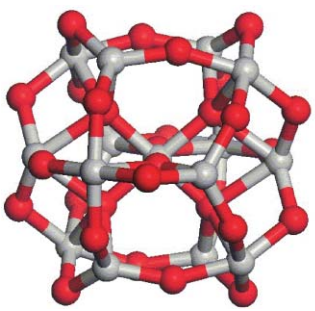


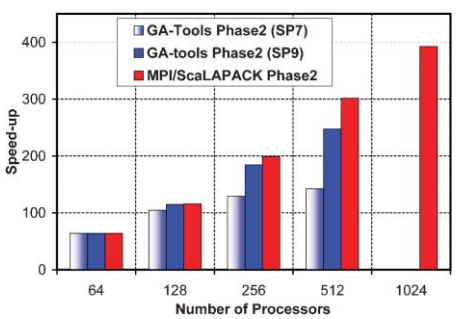
Cover
See Kafui Tay and Fernando Bresme, pp. 1956–1962. Molecular dynamics computer simulation snapshot of the hydrogen bond structure of interfacial water around a passivated gold metal nanoparticle of 3 nm diameter. Image reproduced by permission of Fernando Bresme from *J. Mater. Chem.*, 2006, **16**, 1956.

EDITORIAL



Ground state structure of $(TiO_2)_{15}$

FEATURE ARTICLES



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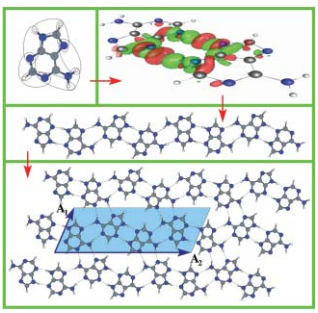

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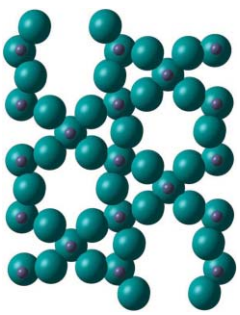
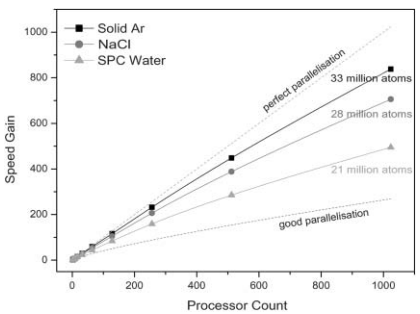
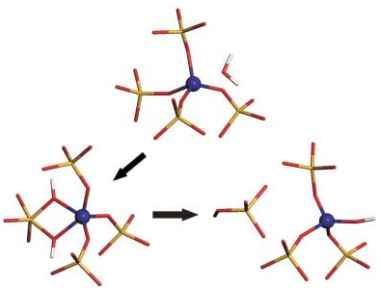
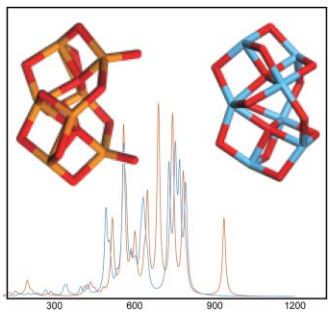






1927

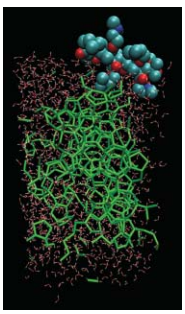


Properties of small TiO_2, ZrO_2 and HfO_2 nanoparticles

S. M. Woodley,* S. Hamad, J. A. Mejías and C. R. A. Catlow

Ground state structures, based on DFT, and infrared spectra are predicted and compared for $(MO_2)_n$, where n = 1 to 8 and M is one of three isovalent cations.

1934

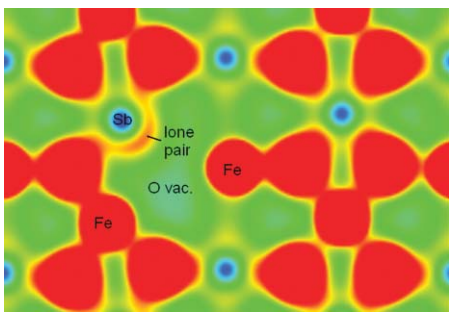


Polydispersity in oligomeric low dosage gas hydrate inhibitors

Robert W. Hawtin and P. Mark Rodger*

This paper presents the first molecular-level study of the influence of tacticity and conformation on the activity of low dosage hydrate inhibitors. PDMAEMA is shown to promote nucleation, with linear conformations generating slower nucleation and growth than helical forms.

1943

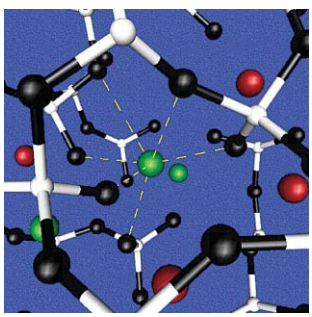


The effect of cation coordination on the properties of oxygen vacancies in $FeSbO_4$

Ricardo Grau-Crespo,* Ibério de P. R. Moreira, Francesc Illas, Nora H. de Leeuw and C. Richard A. Catlow

We investigate the dependence of the oxygen vacancy properties on the cation coordination of the removed oxygen atom in iron antimonate $FeSbO_4$, an important catalyst for the selective oxidation of hydrocarbons.

1950



Structural and electronic properties of modified sodium and soda-lime silicate glasses by Car–Parrinello molecular dynamics

Antonio Tilocca* and Nora H. de Leeuw

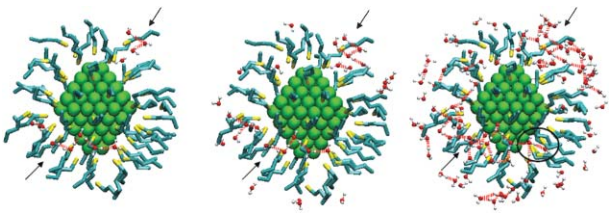
Car–Parrinello molecular dynamics simulations elucidated structural and electronic properties of modified silicate glasses, relevant to the technological applications of these materials; in particular, the local environment of Na and Ca ions has been determined with high accuracy.

1956

Hydrogen bond structure and vibrational spectrum of water at a passivated metal nanoparticle

Kafui Tay and Fernando Bresme*

Molecular Dynamics computer simulations show that gold passivated nanoparticles (~3 nm diameter) in water exhibit weak dewetting, similar to that observed in extended hydrophobic surfaces. The nanoparticle–water interface is characterised by a reduction in the number of hydrogen bonds compared to bulk water and by the existence of OH dangling bonds.

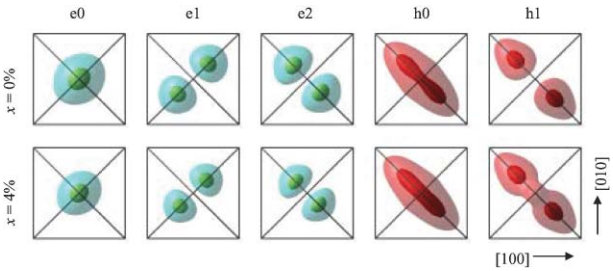


1963

Parallel multi-band k·p code for electronic structure of zinc blend semiconductor quantum dots

Stanko Tomić,* Andrew G. Sunderland and Ian J. Bush

A parallel implementation of the multi-band **k·p** code has been developed for the electronic structure and optical properties calculation of conventional and dilute nitrogen zinc blend semiconductor quantum dots.

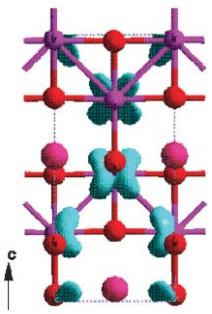


1973

Li sites and phase stability in TiO_2-anatase and Zr-doped TiO_2-anatase

Marina V. Koudriachova* and N. M. Harrison

Doping anatase TiO_2 with zirconium decreases its intercalation potential.

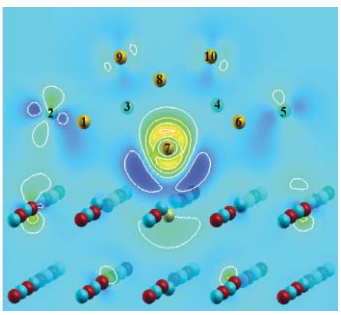


1978

Calculations on the adsorption of Au to MgO surfaces using SIESTA

Rudy Coquet, Graham J. Hutchings, Stuart H. Taylor and David J. Willock*

Au_n (n = 1, 2, and 10) on MgO is stabilised at defect sites. The adsorption of these species at point and extended defects is compared.



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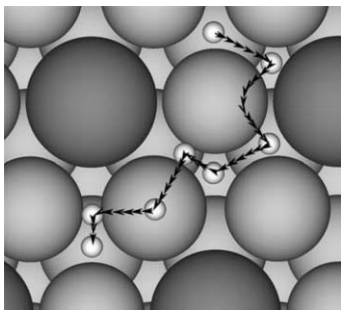
1989

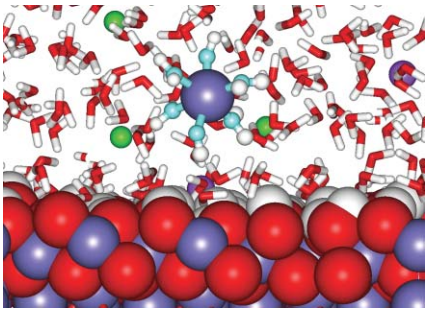


Hydrogen adsorption and diffusion on Pt {111} and PtSn {111}

Joanne Fearon and Graeme W. Watson*

Addition of Sn to the Pt {111} surface results in substantial differences for the mobility of H on the surface. Nudged elastic band calculations show H follows a path that avoids interaction with the Sn atoms.

1997



Molecular dynamics simulations of the interaction between the surfaces of polar solids and aqueous solutions

Dino Spagnoli, David J. Cooke, Sebastien Kerisit and Stephen C. Parker*

Atomistic simulation techniques allow the speciation of metal ion complexes at mineral/electrolyte interfaces to be explored.

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